Reply to Comment on the paper "Pairing mechanism of high-temperature superconductivity: Experimental constraints"

Guo-meng Zhao[1,2,*]
[1]*Department of Physics and Astronomy, California State University, Los Angeles, CA 90032, USA*
[2]*Department of Physics, Faculty of Science, Ningbo University, Ningbo, P. R. China*

In our recent paper entitled "Pairing mechanism of high-temperature superconductivity: Experimental constraints" (to be published in Physica Scripta), we review some crucial experiments that place strong constraints on the microscopic pairing mechanism of high-temperature superconductivity in cuprates. In particular, we show that phonons rather than spin-fluctuation play a predominant role in the microscopic pairing mechanism. We further show that the intrinsic pairing symmetry in the bulk is not d-wave, but extended s-wave (having eight line nodes) in hole-doped cuprates and nodeless s-wave in electron-doped cuprates. In contrast, the author of the Comment (to be published in Physica Scripta) argues that our conclusions are unconvincing and even misleading. In response to the criticisms in the Comment, we further show that our conclusions are well supported by experiments and his criticisms are lack of scientific ground.

In our recent paper [1], we review some crucial experiments that place strong constraints on the microscopic pairing mechanism of high-temperature superconductivity in cuprates. In particular, we show that phonons rather than spin-fluctuation play a predominant role in the microscopic pairing mechanism. We further show that the intrinsic pairing symmetry in the bulk of cuprates is not d-wave, but extended s-wave (having eight line nodes) in hole-doped cuprates and nodeless s-wave in electron-doped cuprates. However, Plakida [2] has raised strong criticisms on these conclusions based on an oversimplified polaronic model and some experimental results that have been misinterpreted. Below we will show that our conclusions are well supported by experiments and the criticisms raised in the Comment are lack of scientific ground.

In the Comment [2], the author first considers the oxygen-isotope effect (OIE) on T_c by taking into account the observed oxygen-isotope effect on the in-plane effective supercarrier mass. He has used the weak-coupling BCS-like formula [Eq. (2) in the Comment] to calculate the doping dependence of the OIE on T_c in $La_{2-x}Sr_xCuO_{4-y}$ (LSCO) on the assumption that the electron-phonon coupling constant λ_{ep} has the same OIE on the in-plane effective supercarrier mass. Actually, Eq. (2) used in the Comment is incorrect. The correct T_c formula in the (bi)polaron theory has the polaronic half bandwidth in front of the exponent rather than the phonon energy [3]. When the correct expression is applied, the theory describes well the doping dependence of the isotope exponents in many cuprate superconductors [3]. Also, the tunneling experiments [4, 5] have consistently shown that λ_{ep} is larger than 2.5 for optimally doped $Bi_2Sr_2CaCu_2O_{8+y}$ (BSCCO). Therefore, the weak-coupling BCS-like formula does not hold in cuprates. A strong-coupling formula has been used to consistently explain the negligible OIE on T_c and substantial OIE on the in-plane effective supercarrier mass in nearly optimally doped BSCCO [6]. In the underdoped regime, superconductivity should be better described by the Bose-Einstein condensation of local pairs in the strong coupling limit [7]. In this case, T_c is essentially proportional to n_s/m^{**}_{ab} (where n_s is the supercarrier density and m^{**}_{ab} is the in-plane effective supercarrier mass), in agreement with the well-known Uemura plot [8]. This implies that the OIE on T_c is essentially proportional to the OIE on m^{**}_{ab}. This scenario can naturally explain why the magnitudes of the exponents for the OIE on both T_c and m^{**}_{ab} increase with the decrease of doping and are even larger than 0.5 in deeply underdoped samples (e.g., $La_{1.94}Sr_{0.06}CuO_{4-y}$) [1, 9]. Therefore, the claim that the polaronic effects cannot explain the doping dependence of the OIE on T_c is lack of scientific ground.

Then the author of the Comment [2] attempts to explain the doping dependence of the OIE on T_c in terms of his own theory based on the $t-J$ model. According to his model [2], $\Delta T_c/T_c = (1/\lambda)\Delta J/J$, where $\lambda = 0.2-0.3$. Since the OIE on J was found to be -0.9% for undoped $YBa_2Cu_3O_6$ (Ref. [10]), the predicted $\Delta T_c/T_c$ for the optimally doped $YBa_2Cu_3O_{6.94}$ should be $-(2.7-4.5)\%$, in disagreement with the measured value of -0.27% (Ref. [11]). In the deeply underdoped regime, $T_c \propto 1/m^{**}_{ab}$ and $1/m^{**}_{ab} \propto J$ within the $t-J$ model, so $\Delta T_c/T_c = \Delta J/J = -(0.6-0.9)\%$, in disagreement with the measured values of $-(5-12)\%$ (Ref. [9]). Therefore, the $t-J$ model cannot explain the doping dependence of the OIE on T_c. Further, the author of the Comment [2] argues that since the site-selective OIE shows that the OIE on T_c mainly contributes from the planar oxygen, the apical oxygen is not important for the pairing. This argument is in parallel with the statement that since the optimally doped $YBa_2Cu_3O_{6.94}$ has a negligible OIE on T_c, phonons are not important to the pairing mechanism. In fact, the site-selective OIE experiment [12] shows that the apical oxygen contributes about 40% of the OIE on m^{**}_{ab} in $YBa_2Cu_3O_{6.94}$. This suggests that the apical oxygen is important to the pairing, in agreement with our argument based on the bulk-sensitive x-ray-absorption experiment [13] on $(Y_{1-x}Ca_x)Ba_2Cu_3O_{7-y}$.

The author of the Comment also criticizes the conclu-

sion about strong coupling to multiple phonon modes revealed by both tunneling [4, 5, 14–17] and angle-resolved photoemission spectra (ARPES) [17, 18]. There are several important facts about the strong coupling features revealed by both tunneling and ARPES data. First, the energies of strong coupling features match very well with those of the phonon modes revealed by the neutron [14] and Raman [15] data. Second, the energies of strong coupling features revealed by tunneling spectra match very well with those of strong coupling features revealed by ARPES [17]. Third, the energies of strong coupling features in different cuprate systems such as LSCO, YBCO, and BSCCO are very similar [14, 17, 18] and nearly independent of doping [19]. Such excellent consistencies unambiguously demonstrate that these strong-coupling features are intrinsic and arise from strong electron-phonon interactions. Furthermore, a detailed review of tunneling, ARPES, and optical experiments has recently been given by Maksimov *et al.* [19]. These authors provide consistent evidence for strong coupling to multiple phonon modes from the tunneling, ARPES, and optical results.

Concerning the spin-fluctuation pairing, we have shown that the magnetic resonance mode revealed by neutron experiments plays a minor role in high-temperature superconductivity [1, 16]. One might argues that since the magnetic resonance mode is only a small fraction of the spin-excitation spectrum [20], its contribution to the electron pairing should be insignificant while the coupling to the whole spin-excitation spectrum may still play an important role in the d-wave pairing. A recent theoretical calculation [21] has shown that strong coupling to the whole spin-excitation spectrum of underdoped $YBa_2Cu_3O_{6.6}$ (measured by neutron scattering) can lead to d-wave high-temperature superconductivity with $T_c = 174$ K and the coupling constant $\lambda_d = 1.39$. It is important to note that the authors of Ref. [21] have used a large renormalized coupling strength $\bar{U}$ (1.59 eV), which is too large compared with that estimated from several other independent experiments (see a recent review article [19]). These experiments consistently show that [19, 20] $\bar{U} < 0.17$ eV. This implies that $\lambda_d < 0.0115$ (since $\lambda_d \propto \bar{U}^2$). Such a small coupling constant cannot lead to high-temperature superconductivity. Further experimental evidence for no magnetic pairing mechanism is that T_c is very insensitive to the magnetic spectral weight, as clearly demonstrated from the neutron data [22] of slightly underdoped $YBa_2Cu_3O_{6.92}$ and slightly overdoped $YBa_2Cu_3O_{6.97}$. The two compounds have almost the same T_c (91-93 K), but the magnetic spectral weight for $YBa_2Cu_3O_{6.97}$ is at least three times smaller than that for $YBa_2Cu_3O_{6.92}$. As pointed out by Maksimov *et al.* [19], the little dependence of T_c on the magnetic spectral weight is incompatible with the magnetic pairing mechanism. On the theoretical ground, recent variational Monte Carlo simulations [23], which are based on an advanced sign-problem-free Gaussian-Basis Monte Carlo algorithm, have shown that the simplest Hubbard model, advocated by Plakida and some other authors, does not account for high-temperature superconductivity.

Another important issue is the intrinsic pairing symmetry in the bulk of superconducting cuprates. Because nearly all the surface and phase-sensitive experiments for both electron- and hole-doped cuprates provide clear evidence for d-wave order-parameter (OP) symmetry [24], the d-wave pairing symmetry has become an indisputable fact to most researchers in the field. However, it is important to note that these surface and phase-sensitive experiments based on planar Josephson tunneling are probing the OP symmetry at surfaces and interfaces, which were found to be underdoped [25, 26]. Since the majority of charge carriers are oxygen-hole bipolarons in the underdoped regime [1] and the OP symmetry of the Bose-Einstein condensate of the oxygen-hole bipolarons is d-wave [27], the phase-sensitive experiments just probe the d-wave OP symmetry of the dominant component. Since the OP symmetry of the Bose-Einstein condensate has nothing to do with the pairing symmetry, the phase-sensitive experiments do not probe the pairing symmetry associated with the pairing interaction. In order to probe the intrinsic pairing symmetry, bulk-sensitive data should be obtained from significantly overdoped samples where the dominant charge carriers are Fermi-liquid-like and the superconducting transition is mean-field-like [1]. Based on the quantitative analyses of many bulk-sensitive experiments (in addition to some bulk- and phase-sensitive experiments such as nonmagnetic pair-breaking effects), we have concluded that the intrinsic pairing symmetry in the bulk of cuprates is not d-wave, but extended s-wave (having eight line nodes) in hole-doped cuprates [28] and nodeless s-wave in electron-doped cuprates [29, 30].

The author of the Comment does not believe the intrinsic pairing symmetry inferred from the bulk and phase-sensitive nonmagnetic pair-breaking effects. He argues against the extended s-wave gap symmetry using the surface-sensitive ARPES and Fourier transform scanning tunneling spectroscopy (FT-STM) experiments. Even surface-sensitive ARPES data of nearly optimally doped BSCCO can be better explained in terms of an extended s-wave gap [17, 28, 31]. The gap along the diagonal direction Δ_D is small (≤ 7 meV) for nearly optimally doped BSCCO [17, 31] but becomes larger in heavily overdoped BSCCO [28, 32]. Furthermore, both surface-sensitive ARPES and FT-STM data of a nearly optimally overdoped BSCCO can also be well explained in terms of an extended s-wave gap with $\Delta_D \simeq 4$ meV (Ref. [31]). The significant uncerntainty in extracting the gap size from the ARPES data in a slightly overdoped and two underdoped BSCCO crystals [33] does not allow one to make distinction between a d-wave gap and an extended s-wave gap with $\Delta_D \leq 4$ meV. In fact, no ARPES data along the diagonal direction were given in this study [33], which

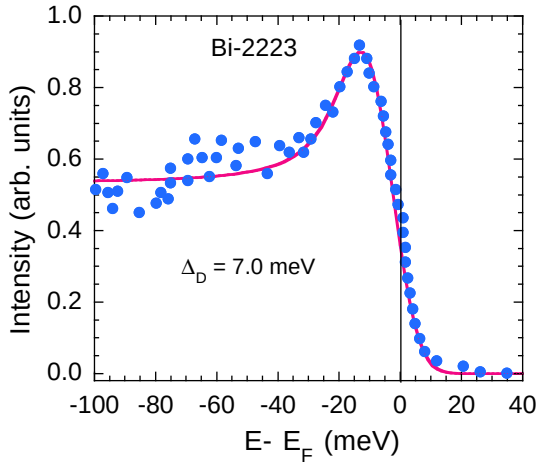

FIG. 1: Photoemission spectrum along the diagonal direction for a nearly optimally doped $Bi_2Sr_2Ca_2Cu_3O_{10+y}$ (Bi-2223). The spectrum was taken with an energy resolution of 10 meV (Ref. [36]). The solid line is the curve calculated with the fitting method of Ref. [34] and the following parameters: Δ_D = 7.0 meV and Γ = 9.0 meV.

makes it harder to draw a definitive conclusion about the gap symmetry from the ARPES data.

In order to further prove our extended s-wave pairing symmetry in hole-doped cuprates, we determine the Δ_D value from some high-resolution ARPES data. The fitting method used in Ref. [34] for extracting the gap size from ARPES data should be the most reliable since the gap sizes extracted from this method match precisely with those independently determined from the FT-STM data [31]. Fig. 1 shows photoemission spectrum along the diagonal direction for a nearly optimally doped $Bi_2Sr_2Ca_2Cu_3O_{10+y}$ (Bi-2223). The spectrum was taken with an energy resolution of 10 meV (Ref. [36]). The solid line is the curve calculated with the method of Ref. [34] and the following parameters: Δ_D = 7.0 meV and Γ = 9.0 meV (where Γ is the electron life-time broadening parameter). It is apparent that the gap size along the diagonal direction is not zero.

In Fig. 2, we show photoemission spectra along the diagonal direction for a nearly optimally doped BSCCO (Fig. 1a) and a heavily overdoped BSCCO (Fig. 1b). The spectra for the nearly optimally doped and heavily overdoped BSCCO crystals were taken with energy resolutions of about 6 meV and 10 meV, respectively [32, 37]. The solid lines are the curves calculated with the following parameters: Δ_D = 6.0 meV and Γ = 6.0 meV for the nearly optimally doped BSCCO; Δ_D = 14 meV and Γ = 18 meV for the heavily overdoped BSCCO. It is striking that Δ_D increases from the increase of doping, in agreement with the earlier ARPES result [35] and break-junction tunneling experiments [28].

In summary, our conclusions of the phonon-mediated pairing mechanism and s-wave pairing symmetry in cuprates are well supported by experiments. The criticisms raised in the Comment [2] are lack of scientific ground although the author of the Comment agrees that there exist polaronic charge carriers and electron-phonon coupling is strong in cuprates.

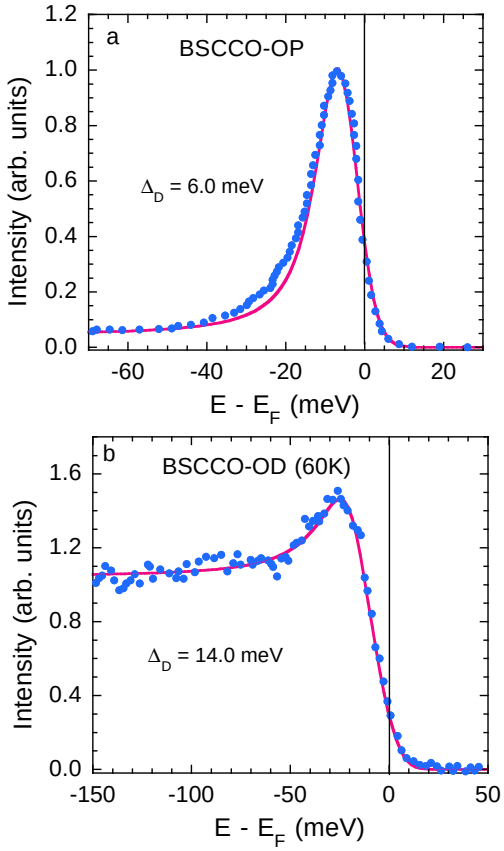

FIG. 2: a) Photoemission spectrum along the diagonal direction for a nearly optimally doped BSCCO. The spectrum was taken with an energy resolution of about 6 meV (Ref. [37]). b) Photoemission spectrum along the diagonal direction for a heavily overdoped doped BSCCO with T_c = 60 K. The spectrum was taken with an energy resolution of about 10 meV (Ref. [32]). The solid lines are the curves calculated with the following parameters: Δ_D = 6.0 meV and Γ = 6.0 meV for the nearly optimally doped BSCCO; Δ_D = 14 meV and Γ = 18 meV for the heavily overdoped BSCCO.

* gzhao2@calstatela.edu

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